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L1 88181 S (COELUT? OR CO ELUT? OR OVERLAP? OR OVER LAP? OR INCOMPLET?(2A)(SEPARAT? OR RESOLV? OR RESOLUT?))
L2 8333 S (COELUT? OR CO ELUT? OR OVERLAP? OR OVER LAP? OR INCOMPLET?(2A)(SEPARAT? OR RESOLV? OR RESOLUT?))/TI,IT,ST
L3 6254 S L1 AND(ISOTOP? OR LABEL? OR ENRICH? OR 13C OR C13 OR(C OR CARBON)(A)13)
L4 606 S L3 AND CHROMATOG?
L5 314 S L2 AND(ISOTOP? OR LABEL? OR ENRICH? OR 13C OR C13 OR(C OR CARBON)(A)13)
L6 901 S L4-5
L7 138 S L6 AND MASS SPECTRO?
L8 8054 S L1(4A)(PEAK OR SIGNAL OR BAND)OR(L1 AND CHROMATOG?(3A)(PEAK OR SIGNAL OR BAND))
L9 145 S L6 AND L8
L10 22 S L6 AND ISOTOP?(2A)(2 OR 3 OR 4 OR TWO OR DUAL OR DOUBLE OR THREE OR TRIPLE OR FOUR OR MULTI OR MULTIPLE OR PLURAL?)
L11 273 S L7,L9-10
L12 200 S L11 NOT PY>1997
L13 1 S L11 NOT L14 AND PATENT/DT AND PY<1999
L14 201 S L12-13

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L14 ANSWER 8 OF 201 CA COPYRIGHT 2003 ACS
AN 126:194586 CA
TI Investigation of HfO+ interference in the determination of platinum in a catalytic converter (cordierite) by inductively coupled plasma **mass** spectrometry
AU Parent, M.; Vanhoe, H.; Moens, L.; Dams, R.
CS Laboratory of Analytical Chemistry, Institute for Nuclear Sciences, Ghent University, Ghent, B-9000, Belg.
SO Talanta (1997), 44(2), 221-230
AB The detn. of Pt in cordierite is subject to strong interference by spectral **overlap** from HfO+ ions with all Pt **isotopes**. Two math. correction methods based on the HfO+Hf+ ratio and a method for the chem. sepn. of Hf based on adsorption **chromatog**. and **isotope** diln. were studied to correct for this interference. Flow infection was used to prevent clogging of the cone orifice. To enhance the sensitivity and thus lower the detection limit, thermospray nebulization was used for sample introduction and the method was compared with pneumatic nebulization. The memory effects were evaluated for both systems. Anal. of artificial solns. (1 ng Pt ml-1) yielded results within 3% of the true value. The Pt content (~50 ng g-1) of a cordierite sample, previously exposed to exhaust gases, could be detd. with precisions of ~10-25% and the results agreed with earlier detns. by other workers.

L14 ANSWER 11 OF 201 CA COPYRIGHT 2003 ACS
AN 126:44528 CA
TI Calibration for **isotope** dilution **mass** spectrometry - description of an alternative to the bracketing procedure
AU Thienpont, Linda M.; Van Niewwenhove, Benedikt; Stoeckl, Dietmar; De Leenheer, Andre P.
CS Laboratoria voor Medische Biochemie en voor Klinische Analyse, Universiteit Gent, Ghent, B-9000, Belg.

SO Journal of Mass Spectrometry (1996), 31(10), 1119-1125
AB A calibration method for **isotope** diln. **mass** spectrometry is presented that fully accounts for non-linearity of calibration functions, caused by the interference of the analyte on the m/z used for measurement of the internal std. and vice versa. In this way, it is also possible to use incompletely **labeled** mols. of analogs with an mass increment of only 1 u for **isotope** diln., on condition that certain restrictions are respected. In addn., the proposed method is less time consuming than bracketing. The method works with the computer-stored full calibration curve and a single calibration point that is measured daily. The calibration curve is constructed from the exptl. detd. mass spectral **overlap** between the unlabeled analyte and the **labeled** internal std. at the m/z values chosen for measurement. Measurement results for samples with unknown analyte concn. are calcd. on the basis of a linear relationship between their ion abundance ratio and that of the daily single calibration point, but cor. by a factor derived from the theor. calibration function. All calcns. are performed with commonly available spreadsheet software. An application is presented for detg. serum uric acid with a candidate gas **chromatog.**/**isotope** diln. **mass** spectrometric ref. method.

L14 ANSWER 13 OF 201 CA COPYRIGHT 2003 ACS
AN 125:236973 CA
TI Determination of lanthanides and actinides in uranium materials by high-performance liquid **chromatography** with inductively coupled plasma **mass** spectrometric detection
AU Roellin, S.; Kopatjtic, Z.; Wernli, B.; Magyar, B.
CS Laboratory for Materials and Nuclear Processes, Paul Scherrer Institute, Villigen-PSI, CH-5232, Switz.
SO Journal of Chromatography, A (1996), 739(1 + 2), 139-149
AB The detn. of Nd, U and Pu by **isotope** diln. anal. is known as the classical method for the calcn. of the burn-up of a nuclear fuel. Numerous isobaric **overlaps** restrict the direct detn. of fission product and actinide **isotopes** by **mass** spectrometry and therefore an extensive chem. sepn. is required. As a 1st step towards the development of a more advanced method for the detn. of fission product **isotopes** in irradiated U fuel, HPLC and inductively coupled plasma **mass** spectrometric (ICP-MS) systems were installed in glove-boxes and all the lanthanides were sepd. by HPLC and detected online by ICP-MS. As high U and Pu concns. strongly suppress the signals of trace elements in ICP-MS, a sepn. method to elute U and Pu 1st was developed. Thus it was possible to det. the **isotopic** compn. of Nd in a high U and Pu matrix. With the same equipment, a method was developed to prevent isobaric **overlaps** in the mass spectrum by sepg. U, Am and Pu.

L14 ANSWER 16 OF 201 CA COPYRIGHT 2003 ACS
AN 125:162658 CA
TI Determination of **isotopic** ratios of L-leucine and L-phenylalanine and their stable **isotope-labeled** analogs in biological samples by gas **chromatography**/triple-stage quadrupole **mass** spectrometry
AU Schweer, Horst; Watzer, Bernhard; Seyberth, Hannsjoerg W.; Steinmetz, Armin; Schaefer, Juergen R.
CS Children's Hospital, Philipps Univ. Marburg, Marburg, 35033, Germany
SO Journal of Mass Spectrometry (1996), 31(7), 727-734
AB A gas **chromatog.**/triple-stage quadrupole **mass** spectrometric (GC/MS/MS) method for measuring very low levels of **enrichment** of [5,5,5-2H3]-L-leucine and [ring-13C6]-L-phenylalanine in plasma and lipoprotein hydrolyzates is described. The amino acids were derivatized to their N-heptafluorobutyryl iso-Bu ester derivs., and the **isotope** ratio was detd. by GC/MS/MS in the neg.-ion chem.-ionization mode. Parent ions were the [M-HF]-1 ions and

fragment ions used for quantification were [P-2HF-C3H7]- (leucine) and [P-HF-OC4H9]- (phenylalanine). The limit of quantification was about 10 pg of the **labeled** compd. **co-eluting** with 20 ng of the endogenous compd. The calibration curves were linear in the investigated range from 0.1% to 100% of the **labeled** compd. In biol. samples, the higher selectivity of GC/MS/MS compared with GC/MS was demonstrated.

L14 ANSWER 20 OF 201 CA COPYRIGHT 2003 ACS
AN 124:75150 CA
TI Multi-element detection of organometals by supercritical fluid **chromatography** with inductively coupled plasma **mass** spectrometric detection
AU Kumar, Uma T.; Vela, Nohora P.; Caruso, Joseph A.
CS Dep. Chem., Univ. Cincinnati, Cincinnati, OH, 45221-0172, USA
SO Journal of Chromatographic Science (1995), 33(11), 606-10
AB Organometal compds. of arsenic, antimony, and mercury are speciated using supercrit. fluid **chromatog.** with inductively coupled plasma **mass** spectrometric (ICP-MS) detection. The multielement capability of ICP-MS for transient signals is examd. by detecting five compds. contg. all three elements in a single **chromatog.** injection. The results obtained are compared with those obtained from flame-ionization detection (FID). Tri-Me arsine is not distinguished from the solvent peak when FID is used because it **coelutes** with the solvent, whereas tri-Me arsine is detected when ICP-MS is used because of its element-selective nature. The detection limits obtained by ICP-MS are 2-3 orders of magnitude lower than those obtained by FID. Detn. and **isotope** abundance is also demonstrated for tri-Ph antimony and di-Ph mercury compds.

L14 ANSWER 23 OF 201 CA COPYRIGHT 2003 ACS
AN 123:274783 CA
TI Separation of precolumn-**labeled** D- and L-amino acids by micellar electrokinetic **chromatography** with UV and fluorescence detection
AU Tivesten, Anna; Folestad, Staffan
CS Department of Analytical and Marine Chemistry, University of Goeteborg/Chalmers University of Technology, Goteborg, S-412 96, Swed.
SO Journal of Chromatography, A (1995), 708(2), 323-37
AB Micellar electrokinetic **chromatog.** (MEKC) was examd. for the sepn. of **labeled** D- and L-amino acids to permit rapid screening of protein amino acid enantiomers in microchem. anal. work. Precolumn chiral derivatization was performed using o-phthaldialdehyde/2,3,4,6-tetra-O- acetyl-1-thio-β-D-glucopyranose (OPA/TATG) reagent and the diastereomers formed were detected by UV or fluorescence detection. Optimization of sepn. buffer pH, ionic strength and surfactant concn. was carried out and was focused on the effective sepn. window available for the resoln. of the amino acid derivs. The effects of added org. modifiers, methanol, acetonitrile and THF, on the relative retention of the derivs. were characterized for the purpose of fine tuning the sepn. selectivity. The resoln. of the derivs. of the D- and L-forms of each protein amino acid was very high (mean value of Rs = 14.3, range 0.8-28), except for aspartic acid and glutamic acid, whose enantiomers could not be resolved at the alk. pH studied. A sepn. of 34 D,L-amino acids in less than 5 min, is demonstrated with only a few **peaks co-eluting**.

L14 ANSWER 31 OF 201 CA COPYRIGHT 2003 ACS
AN 122:247797 CA
TI Online trace **enrichment** of polar pesticides in environmental waters by reversed-phase liquid **chromatography**-diode array detection-particle beam **mass** spectrometry
AU Marce, R. M.; Prosen, H.; Crespo, C.; Calull, M.; Borrull, F.; Brinkman, U.

A. Th.
CS Department of Chemistry, Universitat Rovira i Virgili, Imperial Tarraco 1, Tarragona, 43005, Spain
SO Journal of Chromatography, A (1995), 696(1), 63-74
AB The detn. of a group of pesticides by reversed-phase liq. **chromatog.** (RPLC)-diode array detection, coupled online to particle beam mas spectrometry (MS), is developed for the anal. of different environmental waters. Online trace **enrichment** of 100 mL of sample on a PLRP-S precolumn allows the detn. of most pesticides at levels between 0.2 and 5 μg/L and detection limits in the range 0.05-0.5 μg/L for diode array detection and 0.02-0.5 μg/L for particle beam MS. With real-life samples, a distinct matrix effect is obsd. in particle beam MS detection, which is caused by **coeluting** compds. acting as carriers. This improves analyte detectability and requires std. addn. to be used for quantification. Different river and drinking waters were analyzed, and some pollutants were detected at sub-μg/L levels.

L14 ANSWER 33 OF 201 CA COPYRIGHT 2003 ACS
AN 122:150716 CA
TI Simultaneous analysis of diphenylmethoxyacetic acid, a metabolite of diphenhydramine, and its deuterium-**labeled** stable **isotope** analog in ovine plasma and urine
AU Tonn, George R.; Abbott, Frank S.; Rurak, Dan W.; Axelson, James E.
CS Division of Pharmaceutics and Biopharmaceutics, Faculty of Pharmaceutical Sciences, University of British Columbia, Vancouver, B.C. V6T 1Z3, Can.
SO Journal of Chromatography, B: Biomedical Applications (1995), 663(1), 67-81
AB Diphenylmethoxyacetic acid (DPMA) is a major metabolite of diphenhydramine in monkeys, dogs, and humans. The metabolic fate of diphenhydramine (DPHM) in sheep is not yet well understood; however, preliminary studies have demonstrated the presence of DPMA in the plasma and urine of sheep following an i.v. bolus of DPHM. Our current studies employ the simultaneous i.v. co-administration of DPHM and the stable **isotope** analog of DPHM to investigate the pharmacokinetics of DPHM in sheep. In these studies, in order to investigate the pharmacokinetics of the DPMA metabolite, measurement of both unlabeled and stable-**isotope labeled** DPMA is required. Thus, a stable **isotope** analog of DPMA ([2H10]DPMA) was synthesized, characterized, and purified for use as an anal. std. The quant. method for the gas **chromatog.**-electron-impact **mass** spectrometry (GC-EI-MS) anal. of DPMA and [2H10]DPMA used a single step liq.-liq. extn. procedure using toluene for sample cleanup. The samples were derivatized with N-methyl-N-(tert.-butyldimethylsilyl) trifluoroacetamide. A 1.0-μl aliquot of the prepd. sample was injected into the GC-MS system and quantitated using selected-ion monitoring (SIM). One ion was monitored for each compd., namely, m/z 165 for the internal std. diphenylacetic acid, m/z 183 for DPMA, and m/z 177 for [2H10]DPMA. The ion **chromatograms** were free from **chromatog. peaks co-eluting** with the compd. of interest. The calibration curve was linear from 2.5 ng/mL (limit of quantitation) to 250.0 ng/mL in both urine and plasma. The intra-day and inter-day variabilities of this assay method were within acceptable limits (below 20% at the limit of quantitation and below 10% at all other concns.). This method was used to measure the concn. of DPMA and [2H10]DPMA in plasma and urine samples from a ewe in which equimolar amts. of DPHM and [2H10]DPHM were administered by an i.v. bolus dose via the femoral vein. DPMA appeared to persist longer in the plasma and the urine as compared to DPHM. This method is robust and reliable for the quantitation of DPMA and [2H10]DPMA in biol. samples obtained from sheep (e.g. plasma and urine).

L14 ANSWER 37 OF 201 CA COPYRIGHT 2003 ACS

AN 121:291665 CA
TI **Isotope**-ratio-monitoring gas **chromatography-mass** spectrometry: methods for **isotopic** calibration
AU Merritt, Dawn A.; Brand, W. A.; Hayes, J. M.
CS Department of Chemistry, Indiana University, Bloomington, IN, 47405, USA
SO Organic Geochemistry (1994), 21(6-7), 573-83
AB In trial analyses of n-alkanes, precise detns. of **13C** contents were based on **isotopic** stds. introduced by five different techniques and results were compared. Specifically, org.-compd. stds. were coinjected with the analytes and carried through **chromatog.** and combustion with them; or CO2 was supplied from a conventional inlet and mixed with the analyte in the ion source, or CO2 was supplied from an auxiliary mixing vol. and transmitted to the source without interruption of the analyte stream. Addnl., two techniques were studied in which the analyte stream was diverted and CO2 stds. were placed on a near-zero background. All methods provided accurate results. Where applicable, methods not involving interruption of the analyte stream provided the highest performance (σ = 0.00006 at.% **13C** or 0.06‰ for 250 pmol C as CO2 reaching the ion source), but great care was required. Techniques involving diversion of the analyte stream were immune to interference from **coeluting** sample components and still provided high precision ($0.0001 \leq \sigma \leq 0.0002$ at.% or $0.1 \leq \sigma \leq 0.2$‰).

L14 ANSWER 38 OF 201 CA COPYRIGHT 2003 ACS
AN 121:291664 CA
TI Acquisition and processing of data for **isotope**-ratio-monitoring **mass** spectrometry
AU Ricci, Margaret P.; Merritt, Dawn A.; Freeman, Katherine H.; Hayes, J. M.
CS Departments of Geological Sciences and of Chemistry, Indiana University, Bloomington, IN, 47405, USA
SO Organic Geochemistry (1994), 21(6-7), 561-71
AB Methods are described for continuous monitoring of signals required for precise analyses of **13C**, 18O, and 15N in gas streams contg. varying quantities of CO2 and N2. The quant. resoln. (i.e. max. performance in the absence of random errors) of these methods is adequate for detn. of **isotope** ratios with an uncertainty of one part in 105; the precision actually obtained is often better than one part in 104. This report describes data-processing operations including definition of beginning and ending points of **chromatog. peaks** and quantitation of background levels, allowance for effects of **chromatog.** sepn. of **isotopically** substituted species, integration of signals related to specific masses, correction for effects of mass discrimination, recognition of drifts in **mass** spectrometer performance, and calcn. of **isotopic** δ values. Characteristics of a system allowing off-line revision of parameters used in data redn. are described and an algorithm for identification of background levels in complex **chromatograms** is outlined. Effects of imperfect **chromatog.** resoln. are demonstrated and discussed and an approach to deconvolution of signals from **coeluting** substances described.

L14 ANSWER 45 OF 201 CA COPYRIGHT 2003 ACS
AN 120:3909 CA
TI Determination of the **isotope enrichment** of one or a mixture of two stable **labeled** tracers of the same compound using the complete **isotopomer** distribution of an ion fragment; theory and application to in vivo human tracer studies
AU Vogt, Josef A.; Chapman, Thomas E.; Wagner, David A.; Young, Vernon R.; Burke, John F.
CS Trauma Serv., Massachusetts Gen. Hosp., Boston, MA, 02114, USA
SO Biological Mass Spectrometry (1993), 22(10), 600-12

AB Calcns. of flux rates for stable **isotope** tracer studies are based upon **enrichment** values of an infused tracer. The authors propose the detn. of **enrichment** values by gas **chromatog./mass** spectrometry, which is based on tracer mole fraction and **mass** spectrometer signals, normalized over the total signal of an ion fragment **isotopomer** distribution. The method accounts for **overlap** of the signals of one or two tracers and the tracee, high tracer mole fraction and incomplete **labeling** of the (infused) tracer. For the single and multiple tracer case a linear relationship between tracer mole fraction (from zero to one) and all normalized **mass** spectrometer signals is derived. This linearity over the entire range is demonstrated with a single (1-**13C**)glucose tracer and for mixts. of (1-**13C**)- and (3,3-2H2)tyrosine tracers. The linearity allows detn. of the tracer mole fraction for two tracers, using multiple linear regression. The corresponding calibration can rely on measurements of the pure tracer and tracee compd., without weighing or check for chem. purity. This is compared with a calibration based on tracer/tracee mixts. Ests. for the tracer mole fraction are slightly better if based on a calibration, using std. mixts. In all cases the tracer mole fraction can be detd. with high precision (coeff. of variation <5%) and high accuracy. For tyrosine it is demonstrated that the measurement of seven channels rather than three, for the main **isotopomers**, does not reduce the precision in the prediction of the tracer mole fraction. Equations are also derived to use the tracer mole fraction to est. the endogenous prodn. of the tracee under study conditions, assuming a steady state of the host metab.

L14 ANSWER 54 OF 201 CA COPYRIGHT 2003 ACS
AN 118:204463 CA
TI Comments on "**Isotope** dilution liquid **chromatography/mass** spectrometry using a particle beam interface"
AU Stoeckl, Dietmar
CS INSTAND e.V., Duesseldorf, W-4000/1, Germany
SO Analytical Chemistry (1993), 65(10), 1489
AB A polemic in response to D. Doerge et al. (ibid. 1992, 64, 1212). The accuracy of an **isotope** diln. quantification depends not only on the correct calibration and calcn. procedure, but in the first instance on the accuracy of the exptl. obsd. **isotope** ratios, which itself depends on instrument features and on the actual values obsd. Best accuracy is obtained with analyte/internal std. (IS) ratios of 1. When the ratio tends to zero or infinity, the reliability of the measurement decreases. Further, the accuracy of **isotope** diln. measurements decreases with the increase of spectral **overlap** between analyte and IS. This is shown on analyte/IS mixts., with the following relative intensities on M+/M+1+: analyte 100%/21%, IS 100%/60%, 60%/100%, and 0%/100%.

L14 ANSWER 56 OF 201 CA COPYRIGHT 2003 ACS
AN 118:138967 CA
TI Mass transport and calibration in liquid **chromatography** particle beam **mass** spectrometry
AU Ho, James S.; Behymer, Thomas D.; Budde, William L.; Bellar, Thomas A.
CS Environ. Monitor. Syst. Lab., U.S. Environ. Protect. Agency, Cincinnati, OH, USA
SO Journal of the American Society for Mass Spectrometry (1992), 3(6), 662-71
AB Differences in the designs of two liq. **chromatog.** particle beam **mass** spectrometry systems result in differences in the transport of ammonium acetate and differences in ion abundance-enhancing carrier effects. The effect of mobile phase compn., esp. the proportion of water in the mobile phase, on transport efficiency is described. Instrument detection limits for 12 compds. with two different interface designs are presented. The

calibrations are generally nonlinear explained in terms of mass transport effects and supported by expts. with **isotopically labeled** species that **coelute** with the native species. Summary results of a small multilab. study are presented. Calibration with **isotopically labeled** internal stds. is recommended for real-world environmental samples.

L14 ANSWER 57 OF 201 CA COPYRIGHT 2003 ACS
AN 118:116135 CA
TI Determination of Oltipraz in serum by high-performance liquid **chromatography** with optical absorbance and **mass** spectrometric detection
AU Christensen, Richard G.; Malone, Winfred
CS Chem. Sci. Technol. Lab., Natl. Inst. Stand. Technol., Gaithersburg, MD, 20899, USA
SO Journal of Chromatography, Biomedical Applications (1992), 584(2), 207-12
AB Three methods have been developed for the anal. of Oltipraz in serum. A method suitable for routine use employs spiking with a homologous internal std., off-line solid-phase extn., HPLC sepn., and optical absorbance detection at 450 nm. Method detection limit is about 1 ng/mL. A second method, less susceptible to bias from **co-eluting** interferences, uses a stable **isotope-labeled** internal std., similar extn. and sepn., and detection by thermospray **mass** spectrometry. Method detection limit is about 0.2 ng/mL. A third method was developed which can be used without specially synthesized internal stds. It uses online solid-phase extn., with quantification by comparison with external stds. Method detection limit is about 3 ng/mL. Good agreement was obsd. between these methods and with similar and different methods run in other labs. Calibration curves were linear over the entire range which was investigated, i.e., up to 500 ng/mL. Coeffs. of variation were similar for all three methods, being about 5%.

L14 ANSWER 59 OF 201 CA COPYRIGHT 2003 ACS
AN 118:35393 CA
TI Stable **isotope** tracer analysis by GC-MS, including quantification of **isotopomer** effects
AU Rosenblatt, Judah; Chinkes, David; Wolfe, Marta; Wolfe, Robert R.
CS Metab. Unit, Shriners Burns Inst., Galveston, TX, 77550, USA
SO American Journal of Physiology (1992), 263(3, Pt. 1), E584-E596
AB In metabolic tracer studies it is frequently useful to infuse tracers that are differently **labeled** variants of the same mol. These tracers are known as **isotopomers**. Anal. of the **enrichment** of each **isotopic** analog can be accomplished by gas **chromatog.-mass** spectrometry (GC-MS). However, the raw GC-MS data must be cor. to give the information required. This paper addresses how to transform the raw GC-MS data, consisting of relative abundance ratios at specific ion masses, into relative molar ratios of tracer and tracee mols. Several correction factors are necessary. First, the background must be measured and cor. for, since it is always present in the sample. Second, the abundances in the spectrum of the **labeled** mol. are different from those in the unlabeled mol., and this proportionality skew is cor. A third correction factor accounts for the **overlapping** spectra of **two** or more **isotopomers** that cannot be measured independently. The final correction removes the double vision effect that may appear in some spectra due to the presence of (M - H)+ species.

L14 ANSWER 60 OF 201 CA COPYRIGHT 2003 ACS
AN 118:18824 CA
TI Analysis of oligosaccharides by on-line high-performance liquid **chromatography** and ion-spray **mass** spectrometry
AU Suzuki-Sawada, Jun; Umeda, Yoshihisa; Kondo, Akihiro; Kato, Ikunoshin

CS Biotechnol. Res. Lab., Takara Shuzo Co. Ltd., Otsu, 520-21, Japan
SO Analytical Biochemistry (1992), 207(2), 203-7
AB Oligosaccharides were analyzed by a combination of HPLC and **mass** spectrometry (MS). First, oligosaccharides **labeled** with 2-aminopyridine were studied to see if they could be analyzed by MS under the conditions used for sepn. by HPLC. Pyridylamino (PA)-oligosaccharides could be analyzed under these conditions, although the mass spectra were affected. Then, liq. **chromatog.-mass** spectrometry was used to analyze a PA-oligosaccharide mixt. derived from human IgG. The PA-oligosaccharides were sepd. on a reversed-phase column and mass-analyzed directly. The obsd. mol. wts. were close to or identical to those expected from the structures, which were estd. from the elution position on HPLC. This method is rapid and simple, as the **mass** spectrometer can give the accurate mol. wt. of each PA-oligosaccharide in one **chromatog.** run, even if the HPLC sepn. is **incomplete**. This method can be used to extend the so-called two-dimensional mapping of PA-oligosaccharides. The structure can be studied in greater detail by tandem MS.

L14 ANSWER 64 OF 201 CA COPYRIGHT 2003 ACS
AN 116:227360 CA
TI **Isotope** dilution liquid **chromatography/mass** spectrometry using a particle beam interface
AU Doerge, Daniel R.; Burger, Mike W.; Bajic, Steve
CS Dep. Environ. Biochem., Univ. Hawaii, Manoa, HI, 96822, USA
SO Analytical Chemistry (1992), 64(11), 1212-16
AB The use of a particle beam (PB) interface for quantitation by **isotope** diln. LC/MS was investigated. **Coelution** of single-**labeled** internal stds. (IS) with native compds. caused enhancement of the IS signal. The magnitude of enhancement for [3-13C1]caffeine was affected by several exptl. parameters, but no differences were obsd. in the 12C/**13C** response ratios under these conditions or upon analyte introduction via a gas **chromatog.** (GC) interface. No elution enhancement was obsd. with [1,3,7-13C3]caffeine, demonstrating that mass transfer effects and chem. complex formation do not affect PB transmission efficiency. Spectral **overlap** between native analyte and IS peaks and nonlinear detector response cause the obsd. **coelution** enhancement. These results confirm that PB/LC/MS does not have inherent limitations for use in **isotope** diln. expts. as they have been performed by GC/MS. An equation was derived that permits accurate calcn. of **isotope** diln. results using a single- or multiple-**labeled** IS. Application of this equation could allow expansion of the **isotope** diln. technique performed by PB/LC/MS or GC/MS to include single-**labeled** IS compds. without the ned for nonlinear regression anal. of calibration curves. The method was used for detg. caffeine in coffee products.

L14 ANSWER 66 OF 201 CA COPYRIGHT 2003 ACS
AN 116:200709 CA
TI Determination of geosmin in water by enantioselective gas **chromatography**
AU Korth, Wolfgang; Bowmer, Kathleen H.; Ellis, John
CS Div. Water Resour., CSIRO, Griffith, 2680, Australia
SO Journal of High Resolution Chromatography (1991), 14(10), 704-7
AB Enantioselective gas **chromatog.** enables the use, for the 1st time, of (+)-geosmin [applied via com. (±)-geosmin] as the internal std. for the detn. of (-)-geosmin, with detection being either by FID (flame ionization detection) or MID (multiple ion detection). The latter reduces the risk of errors created by **peak overlap**. These risks are reduced even further by using a D-**labeled** geosmin as the internal std. The latter has the further advantage that it may be added at the time of sampling rather than the time of anal., when the (-)-**labeled** std. compensates perfectly for losses of

natural (-)-geosmin by biodegrdn., volatilization, etc., during sample storage. When a **labeled** internal std. is used, the chiral column offers the further advantage that the complete sepn. of (-)-geosmin and (-)-geosmin-d3 means there is no need to correct.

L14 ANSWER 67 OF 201 CA COPYRIGHT 2003 ACS
AN 116:187285 CA
TI Relative response ratios for **dual-isotope** measurements via **coelution** and GC/MS
AU Thomas, Lawrence C.; Weichmann, Walter
CS Dep. Chem., Seattle Univ., Seattle, WA, 98122, USA
SO Talanta (1992), 39(3), 201-6
AB **Dual-isotope** internal std. measurements by GC/MS which mimic **isotope** diln. may suffer from nonlinear response relations, irreproducibilities or unduly large uncertainties because of variations in ionization efficiencies for the resp. **isotopic** forms in the MS source. Such variations may sometimes be avoided via extensive pretreatments, high resoln. GC sepns. and careful control of instrumental parameters. However, an alternative approach is feasible which instead exploits advantages of decreasing GC resoln. By forcing both forms of each analyte to **coelute**, their relative ionization efficiencies in the MS source should be nearly const., thereby effectively allowing for const. relative sensitivities over several orders of magnitude in concn. Thus, const. relative response ratios, required for internal std. calcns., may be attained as a consequence of dramatically lowered GC resoln. **Coelution** results described herein show linear relative sensitivity relations over much broader ranges than obsd. for corresponding conventional calibrations with sepd. components. **Coelution** methods for **dual-isotope** GC/MS detns. are compatible with internal std. calcns. and thereby offer a powerful alternative to the conventional approach of requiring expensive and labor-intensive addnl. pretreatments and sepns. to assure resoln. of measured eluates.

L14 ANSWER 69 OF 201 CA COPYRIGHT 2003 ACS
AN 116:165543 CA
TI Alternating RF/d.c. isolations for quantitation with **coeluting** internal standards in gas **chromatography**/ion trap **mass** spectrometry
AU Kleintop, Brent L.; Yost, Richard A.; Abolin, Craig R.
CS Dep. Chem., Univ. Florida, Gainesville, FL, 32611-2046, USA
SO Journal of the American Society for Mass Spectrometry (1992), 3(1), 85-8
AB A new ion trap scan function for gas **chromatog./mass** spectrometry (GC/MS) quantitation is described that employs alternating mass-selective storage (rf/d.c. isolation) of ions from an analyte and its **coeluting isotopically labeled** internal std. This scan includes two sep. ionization/isolation/mass anal. sequences within the same scan function, each optimized for either the analyte or the internal std. This results in alternating between analyzing the analyte and the internal std. during their **coelution**. The method is conceptually similar to using two different scan functions to analyze either the analyte or the internal std. in alternating scans; however, it is much faster because it eliminates the slow procedure of continuously downloading alternating scan functions from disk. This allows more data points to be obtained over a GC peak, resulting in more reproducible GC peak profiles as well as better sensitivity and precision. Results of calibration curves spanning four orders of magnitude (0.5 pg to 5 ng injected on column) obtained by using this method give excellent linear correlations ($r^2 > 0.9990$) and precision (relative std. deviations of triplicate injections <10%).

L14 ANSWER 70 OF 201 CA COPYRIGHT 2003 ACS

AN 116:143099 CA
TI Quantitative measurements via **co-elution** and **dual-isotope** detection by gas **chromatography-mass** spectrometry
AU Thomas, Lawrence C.; Weichmann, Walter
CS Dep. Chem., Seattle Univ., Seattle, WA, 98122, USA
SO Journal of Chromatography (1991), 587(2), 255-62
AB **Dual-isotope** measurements by gas **chromatog.-mass** spectrometry (GC-MS) which mimic **isotope** diln. may suffer from irreproducibilities or unduly large uncertainities because of variations in ionization efficacies for the resp. forms in the MS source. Such variations are sometimes avoided via extensive pretreatments and high-resoln. GC sepns. However, in some circumstances, an alternative approach is feasible which instead exploits the advantages of decreasing GC resoln. By forcing both forms of each analyte to **co-elute**, their ionization efficacies in the MS source will be virtually identical, thereby allowing for highly reproducible relative response ratios to be attained despite dramatically lowered GC resoln. The **co-elution** results described here are nearly as precise as results from moderate-resoln. sepns. in the absence of interferents. Thus, **dual-isotope** GC-MS measurements with **co-elution** of the target analytes and their resp. **isotopically labeled** internal stds. offer a powerful alternative to the conventional approach of requiring expensive and labor-intensive addnl. pretreatments and sepns.; however, the effects of interferences may be exacerbated by the forced **co-elution** and must also be considered.

L14 ANSWER 72 OF 201 CA COPYRIGHT 2003 ACS
AN 116:33682 CA
TI Measurements using gas **chromatography** with **coelution** and **dual-isotope** atomic emission detection
AU Thomas, Lawrence C.; Ramus, Terry L.
CS Dep. Chem., Seattle Univ., Seattle, WA, 98122, USA
SO Journal of Chromatography (1991), 586(2), 309-13
AB **Dual-isotope** measurements by gas **chromatog.** (GC)-at. emission detection (AED) may enhance results for quant. analyses. Adding a known amt. of an **isotopically labeled** form of target analytes in each sample can compensate for irreproducibilities or uncertainties assocd. with sample pretreatments and sample loading. Similarly, fluctuations in AED temps., flows and interferants can be compensated via the added **labeled** forms if each target analyte and its **isotopically labeled** form **coelute**. Under these conditions they are subject to identical excitation environments and are measured from the same viewed vols. Consequently, improved quant. results may be attained by **coelution** in GC-AED methods which mimic **isotope** diln.

L14 ANSWER 79 OF 201 CA COPYRIGHT 2003 ACS
AN 115:225534 CA
TI The matrix effect in particle beam liquid **chromatography/mass** spectrometry and reliable quantification by **isotope** dilution
AU Brown, F. Reber; Draper, William M.
CS Hazardous Mater. Lab., Berkeley, CA, 94704, USA
SO Biological Mass Spectrometry (1991), 20(9), 515-21
AB The transport efficiency of the particle beam liq. **chromatog./mass** spectrometer interface is influenced by analyte concn. contributing to a widely reported nonlinearity. In this work, **coeluting**, **isotope-labeled** internal stds. were investigated as carriers to improve the transport efficiency and linearity. Three styrene metabolites-mandelic, phenylglyoxylic and hippuric acids-and their pentadeutero analogs were sepd. by reversed-phase liq. **chromatog.** (LC) with an ammonium acetate-acetonitrile mobile phase. Selected pos. ions produced by electron ionization were monitored to generate particle beam LC/**mass** spectrometry

(MS) calibration curves. Particle beam LC/MS not only is nonlinear, but also is subject to a matrix effect presumably by the same mechanism responsible for nonlinearity. **Coeluting**, **isotope-labeled** internal stds. were ineffective at linearizing the particle beam liq. **chromatog./mass** spectrometer detector response. **Isotope** diln. quantification, however, compensates for variable transport efficiencies, linearizes calibration and compensates for the matrix effect, affording reliable quantification of the styrene metabolites.

L14 ANSWER 81 OF 201 CA COPYRIGHT 2003 ACS
AN 115:112965 CA
TI Determination of ethylenethiourea in crops using particle beam liquid **chromatography/mass** spectrometry
AU Doerge, Daniel R.; Miles, Carl J.
CS Dep. Environ. Biochem., Univ. Hawaii, Honolulu, HI, 96822, USA
SO Analytical Chemistry (1991), 63(18), 1999-2001
AB Several food crops (lettuce, apple, banana, papaya) were analyzed for residues of ethylenethiourea (ETU), a suspect thyroid and liver carcinogen present in EBDC fungicides, by using a com. particle beam (PB) LC (Omni PAX 500 column with 5% MeCN in H2O)/MS method. The PB/LC/MS detection limits for ETU in crops (5 ppb, 1.25 ng) are comparable to those obtained by LC with electrochem. detection. Spectra obtained from crop samples contg. as little as 5 ng ETU were matched with the NBS library ref. EI spectrum. **Isotopically labeled** ETU was used as an internal std. for quantitation and detn. of recoveries. No enhancement of mol. ion signal intensity from unlabeled ETU was obsd. upon **coelution** with the **isotopically labeled** variant. This MS method permits detection of ETU with increased selectivity without compromising sensitivity.

L14 ANSWER 94 OF 201 CA COPYRIGHT 2003 ACS
AN 112:15863 CA
TI Development and validation of a liquid **chromatographic-mass** spectrometric assay for the determination of sumatriptan in plasma
AU Oxford, J.; Lant, M. S.
CS Biochem. Pharmacol. Div., Glaxo Group Res. Ltd., Ware/Hertfordshire, SG12 0DP, UK
SO Journal of Chromatography (1989), 496(1), 137-46
AB Sumatriptan succinate is a novel compd. currently in development for the acute treatment of migraine. During early studies in man a sensitive and selective assay was required, which had to be developed rapidly, to det. plasma concns. following an i.v. infusion. Thermospray liq. **chromatog.-mass** spectrometry combined with the advanced automated sample processor was selected to achieve this. Although the assay was required quickly criteria for intra- and inter-assay accuracies and precisions of ±10% had to be achieved. These were obtained only by using a **co-eluting** deuterium-**labeled** internal std. Attempts to use a homolog as an internal std., which did not **co-elute** with sumatriptan, gave inferior results. The assay was linear over the calibration range 2-50 ng/mL with a limit of quantification of 2 ng/mL. The application of the technique to the anal. of samples from a volunteer study is demonstrated.

L14 ANSWER 95 OF 201 CA COPYRIGHT 2003 ACS
AN 111:166678 CA
TI Determination of unlabeled and 13C6-**labeled** moricizine in human plasma using thermospray liquid **chromatography-mass** spectrometry
AU Pieniaszek, Henry J., Jr.; Shen, Huey Shin L.; Garner, Dennis M.; Page, Gary O.; Shalaby, Lamaat M.; Isensee, Robert K.; Whitney, Charles C., Jr.
CS Metab. Pharmacokinet. Sect., Du Pont Pharm., Newark, DE, 19714, USA

SO Journal of Chromatography (1989), 493(1), 79-92
AB Moricizine-HCl is an orally effective antiarrhythmic agent currently marketed in the Soviet Union and undergoing clin. testing in the United States. To facilitate the simultaneous anal. of unlabeled and 13C6-**labeled** moricizine in human plasma, a specific and sensitive method employing liq.-liq. extn. followed by thermospray liq. **chromatog.-mass** spectrometry (LC-MS) was developed. Plasma samples, after addn. of [2H11]moricizine as an internal std., were extd. into methylene chloride under alk. conditions. Exts. were evapd., reconstituted with mobile phase, and **chromatographed** on an ODS column. The LC mobile phase consisted of MeOH-0.1M NH4OAc contg. 0.2% triethylamine (65:35) and it was used at a flow-rate of 1.5 mL/min. Under these conditions, moricizine and [11C6]moricizine **coeluted** at 1.2 min, while [2H11]moricizine eluted slightly earlier. The MS system consisted of a Finnigan 4600 TSQ and a Vestec thermospray interface. Selected ions at m/z 428, 434, and 439 were scanned at 0.2 s per ion. Over a plasma concn. range of 10-800 ng/mL, intra-day precision ranged 1.8-13.3% and intra-day accuracy ranged 1.9-15.8%. This method was successfully used to assay human plasma samples from a pilot moricizine bioavailability study in which tablets and soln. contg. moricizine-HCl and [13C6]moricizine, resp., were simultaneously administered.

L14 ANSWER 103 OF 201 CA COPYRIGHT 2003 ACS
AN 110:187383 CA
TI Combined **chromatographic-isotopic** dilution analysis of fecapentaenes in human feces
AU Peters, John H.; Nolen, Harold W., III; Gordon, G. Ross; Bradford, Wallace W., III; Bupp, James E.; Reist, Elmer J.
CS Life Sci. Div., SRI Int., Menlo Park, CA, 94025, USA
SO Journal of Chromatography (1989), 488(2), 301-13
AB Fecapentaene-12 (FP-12) and fecapentaene-14 (FP-14) are genotoxic unsatd. ether lipids produced by colonic bacteria in man. It was developed and applied to feces collections from normal volunteers direct **isotopic** diln. procedures using tritium-**labeled** (at C5) FP-12 and FP-14 for measuring these compds. FPs were recovered from feces by solvent extn., silica cartridge clean-up and anal. liq. **chromatog.** Low levels of FP-12 and FP-14 (<0.1 to 2.4 μg/g of freeze-dried feces) were obsd. Identity of **chromatog. peaks** was established by **coelution** and by UV absorption spectra obtained via photodiode array scanning. Two unknown peaks were tentatively identified from absorption spectra as closely related compds. with increased (hexaene) or decreased (tetraene) no. of double bonds. Levels of FPs increased after incubation of feces at 37° for 96 h under anaerobic conditions and pre-FP-12 and pre-FP-14 peaks were obsd., which showed identical spectra with authentic FPs. These were interpreted to be isomeric forms of the all-trans-[3H]FPs used for the **isotopic** diln. anal. Total FPs (including pre-FP) yielded a range of 0.3-80 μg FP-12 and 2.8-44 μg FP-14 per g of freeze-dried feces from the study group.

L14 ANSWER 107 OF 201 CA COPYRIGHT 2003 ACS
AN 109:186764 CA
TI Interference of 3-hydroxyisobutyrate with measurements of ketone body concentration and **isotopic enrichment** by gas **chromatography-mass** spectrometry
AU Des Rosiers, Christine; Montgomery, Jane A.; Desrochers, Sylvain; Garneau, Michel; David, France; Mamer, Orval A.; Brunengraber, Henri
CS Dep. Nutr., Univ. Montreal, Montreal, QC, H3C 3J7, Can.
SO Analytical Biochemistry (1988), 173(1), 96-105
AB Concns. and 13C2 molar percent **enrichments** of blood R-3-hydroxybutyrate and acetoacetate are measured by selected ion monitoring gas **chromatog.-mass**

spectrometry. Samples are treated with NaB2H4 to reduce unlabeled and **labeled** acetoacetate to corresponding 2H-**labeled** RS-3-hydroxybutyrate species. Only the gas **chromatog**. **peak** for the tert-butyldimethylsilyl deriv. of 3-hydroxybutyrate needs to be monitored. The various compds. are quantitated by using an internal std. of RS-3-hydroxy-[2,2,3,4,4,4-2H6]butyrate. Concns. of ketone bodies are obtained by monitoring the m/z 159-163 fragments of tert- butyldimethylsilyl derivs. of **labeled** and unlabeled 3-hydroxybutyrate species. High correlations were obtained between ketone body concns. assayed (1) enzymically with R-3-hydroxybutyrate dehydrogenase and (2) by gas **chromatog**.-**mass** spectrometry. The limit of detection is ~10 nmol of substrate in blood samples. The current practice of monitoring the m/z 275-281 fragments overests. the concn. of endogenous R-3-hydroxybutyrate, due to **coelution** of 3-hydroxyisobutyrate, a valine metabolite. The method presented is used to measure ketone body turnover in vivo in 24-h-fasted dogs.

L14 ***ANSWER 111 OF 201*** CA COPYRIGHT 2003 ACS
AN 109:86394 CA
TI **Mass** spectrometry/**mass** spectrometry of prostaglandins: Daughter ion spectra of derivatized and **isotope-labeled** E and D prostanoids
AU Strife, Robert J.; Simms, J. R.
CS Corp. Res. Div., Procter and Gamble Co., Cincinnati, OH, 45239-8707, USA
SO Analytical Chemistry (1988), 60(17), 1800-7
AB The daughter ion spectra of parent ions produced by electron ionization of 4 derivatized prostaglandins (PG's) and 8 deuterated analogs were obtained on a sector **mass** spectrometer of BE configuration (reversed-geometry magnetic sector/elec. sector). Daughter ions were obsd. under unimol. and collisionally activated dissocn. conditions (6-keV lab. energy) in the 2nd field-free region. The various parent ions showed 2 classes of fragmentation: (1) deriv.-specific and (2) backbone-specific. The deuterium **labels** provided evidence for proposed fragmentation pathways of parent ions. **Isotope labeling** also resolved certain **overlapping** daughter ions obscured by kinetic energy release in the spectra of unlabeled compds. Use of this information to develop a systematic rationale for choosing parent ion-daughter ion pairs for selected reaction monitoring of PG's in biol. fluids by gas **chromatog**./**mass** spectrometry/**mass** spectrometry is discussed.

L14 ANSWER 129 OF 201 CA COPYRIGHT 2003 ACS
AN 104:65313 CA
TI Simultaneous determination of glucose turnover, alanine turnover, and gluconeogenesis in human using a **double** stable-**isotope-labeled** tracer infusion and gas **chromatography-mass** spectrometry analysis
AU Martineau, A.; Lecavalier, L.; Falardeau, P.; Chiasson, J. L.
CS Res. Lab. Prostaglandins Mass Spectro., Clin. Res. Inst. Montreal, Montreal, QC, H2W 1R7, Can.
SO Analytical Biochemistry (1985), 151(2), 495-503
AB A new method was developed and validated for measuring simultaneously glucose turnover, alanine turnover, and gluconeogenesis in humans in steady and nonsteady states by using a **double** stable-**isotope-labeled** tracer infusion and gas **chromatog**.-**mass** spectrometry anal. The method is based on the concomitant infusion and diln. of D-[2,3,4,6,6-2H5]glucose and L-[1,2,3-13C3]alanine. The choice of the tracers was on the basis of minimal **overlap** between the ions of interest and those arising from natural **isotopic** abundances. Alanine was chosen as the gluconeogenic substrate because it is the major gluconeogenic amino acid extd. by the liver and, with lactate, constitutes the bulk of the gluconeogenic precursors. The method was validated by comparing the results obtained during simultaneous

infusion of trace amts. of both stable **isotope-labeled** compds. with the radioactive tracers (D-[3-3H]gluicose and L-[1,2,3-14C3]alanine) in a normal and diabetic subject; the radiolabeled tracers were used as the accepted ref. procedure. A slight overestn. of glucose turnover (7.3 vs. 6.8 in normal and 10.8 vs. 9.2 μmol/kg min in diabetic subject) was noticed when the stable **isotope-labeled** tracers were used. For the basal turnover rate of alanine, similar values were obtained in both methods (6.2 μmol/kg min). For gluconeogenesis, higher values were obsd. in the basal state with the stable **isotopes** (0.42 vs. 0.21 μmol/kg min): however, these differences disappeared in the postprandial period after the ingestion of a mixed meal. Despite those minor differences, the overall correlation with the ref. method was excellent for glucose turnover (r = 0.87) and gluconeogenesis (r = 0.86). The **double** stable **isotope-labeled** tracer technique is a reliable, safe, and acceptable method to evaluate those 3 metabolic processes in humans in a single expt.

L14 ANSWER 135 OF 201 CA COPYRIGHT 2003 ACS
AN 103:84393 CA
TI Analysis of deuterium **labeled** blood lipids by chemical ionization **mass** spectrometry
AU Rohwedder, William K.; Emken, Edward A.; Wolf, Darhal J.
CS North. Reg. Res. Cent., U.S. Dep. Agric., Peoria, IL, 61604, USA
SO Lipids (1985), 20(5), 303-11
AB A quant. anal. method has been developed to analyze Me esters of blood fatty acids derived from human subjects fed deuterium-**labeled** fats. The gas **chromatog**. (GC)-**mass** spectroscopy computer method provides for the anal. of the fed deuterium-**labeled** fatty acids, the naturally occurring blood fatty acids and new fatty acids formed by chain elongation or shortening of the fed **labeled** fats. Approx. 20 fatty acids 16, 17, 18 and 20 carbon chain acids were analyzed with a relative std. deviation of 0.02 at the microgram level and a sensitivity of less than one nanogram. The method uses capillary GC to sep. the fatty acid esters and isobutane chem. ionization **mass** spectrometry with multiple ion detection to det. the **isotopic** constituents of the GC peaks. The technique provides for the detn. of **overlapping** GC **peaks labeled** with 2, 4 and 6 deuterium atoms and makes extensive use of computers both for data acquisition and processing.

L14 ANSWER 163 OF 201 CA COPYRIGHT 2003 ACS
AN 94:99086 CA
TI Experiments on the carrier effect in quantitative **mass** spectrometry of steroids
AU Reiffsteck, A.; Dehennin, L.; Scholler, R.
CS Fond. Rech. Hormonol., Paris, 75014, Fr.
SO Advances in Mass Spectrometry (1980), 8A, 295-304
AB The carrier effect in gas **chromatog.-mass** spectroscopy (GC-MS) appears to be a combined effect, generated on the GC column and in the ion source, and each having sep. similar intensities. The measurement of the **isotopic** distribution of a deuterium-**enriched** compd. by GC-MS with a quadrupole mass filter provides results with good precision, but as these deuterium-**labeled** compds. can act as carriers for their corresponding unlabeled analogs, these results must deviate from the accurate values. The **isotopic** relative responses of all the steroids studied here are not influenced by the presence of interfering compds. which **coelute** or arrive at the same time in the ion source. Therefore, quant. **mass** spectrometry with an **isotopic** internal std. will give more reliable results than with an isomeric internal std. in so far as quant. **mass** spectrometry assocd. with capillary column gas **chromatog**. is concerned.

L14 ANSWER 181 OF 201 CA COPYRIGHT 2003 ACS
AN 81:72306 CA
TI Principal-component analysis applied to combined gas **chromatographic- mass** spectrometric data
AU Davis, James E.; Shepard, Allan; Stanford, Nancy; Rogers, L. B.
CS Dep. Chem., Purdue Univ., West Lafayette, IN, USA
SO Analytical Chemistry (1974), 46(7), 821-5
AB Principal-component anal. provides a relatively rapid means for detg. if there are 2 or more components in a single **chromatog. peak** when using the equivalent of a multichannel detector. For a 2-component system, changes in the shape of the plot for the scalars of the 2 major vectors were examd. as functions of the extent of the **overlap** of the distributions, the relative amts. of the 2 components, and the tailing of peaks. The presence of a 2nd component was easy to detect, both in simulations that were noise-free and in many of those to which 10% noise had been added. Some of the same characteristics were found in **overlapped chromatog. peaks** for masses 44 and 45 for the **isotopic** C species of CO2 and for a mixt. of n-hexane and n-heptane for which 6 masses, that intentionally did not include those for the mol. ions, were used.

L14 ANSWER 190 OF 201 CA COPYRIGHT 2003 ACS
AN 69:63889 CA
TI Retention behavior of compounds containing **isotope** by application of an **isotope** scan method within a combination of capillary gas **chromatography** and **mass** spectroscopy
AU Schomburg, G.; Henneberg, D.
CS Max-Planck-Inst. Kohlenforsch., Muelheim/Ruhr, Fed. Rep. Ger.
SO Chromatographia (1968), (1-2), 23-31
AB The sepn. efficiency of capillary columns ~100,000 effective theoretical plates for a 100 m. 0.25 mm. internal diam. column is sufficient for the sepn. of D **labeled** compds. from the corresponding unlabeled compds. By means of the mentioned column doubly **labeled** hydrocarbons can be sepd. completely from undeuterated mols. without difficulties. The mentioned sepn. efficiency is not sufficient for the investigation of the influence of the positions of the D atoms or the complete sepn. of 12C/**13C** or 10B/11B systems. By application of an **isotope**-scan-method the profiles of **overlapped peaks** obtained from **incomplete** sepns. of **isotopic** mols. can be recognized. This can only be done by using a capillary gas **chromatographymass** spectrometer-combination because of the very small influence of **isotopic** effects on the retention data. By this method orders of elution of mols. contg. the different **isotopes** mentioned could be detd. 25 references.

L14 ANSWER 195 OF 201 CA COPYRIGHT 2003 ACS
AN 65:33722 CA
OREF 65:6284a-b
TI High-resolution mass spectra of compounds separated by capillary columns: a plate scan technique
AU Henneberg, Dieter
CS Max-Planck Inst., Mulheim-Ruhr, Germany
SO Anal. Chem. (1966), 38(3), 495-6
AB A combination of a gas **chromatograph** and a **mass** spectrometer permits sepn. and **enrichment** of individual components of mixts. and measurement of their mass spectra directly from the effluent of the capillary column. The **mass** spectrometer inlet system, the **chromatographic** capillary column, connection device, **mass** spectrometer, and flame ionization detector are described and diagrammed. Particular emphasis is given to the importance of the connection of the capillary columns to the **mass** spectrometer. Use of the

combination is illustrated with the analysis of a mixt. of C6H6 and Et propionate. The gas peak is unsym., 1.5 times as wide as it should be, indicating partial **overlap** of the 2 components. The high resolution of the **mass** spectrometer not only gives the elemental compn. of the ions, but separates the 2 spectra. Moreover, if the plate is moved vertically continuously during the emergence of the peak, the 2 spectra are obtained individually, that of the C6H6 appearing earlier.

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